Variational Approach to the Spin-boson Model With a Sub-Ohmic Bath

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The influence of dissipation on quantum tunneling in the spin-boson model with a sub-Ohmic bath is studied by a variational calculation. By examining the evolution of solutions of the variational equation with the coupling strength near the phase boundary, we are able to present a scenario of discontinuous transition in sub-Ohmic dissipation case in accord with Ginzburg-Landau theory. Based on the constructed picture, it is shown that the critical point found in the general way is not thermodynamically the critical point, but the point where the second energy minimum begins to develop. The true cross-over point is calculated and the obtained phase diagram is in agreement with the result of numerical renormalization group calculation.

PACS numbers: 03.65.Yz, 03.65.Xp, 73.40.Gk

I. INTRODUCTION

The spin-boson model is an important toy model for investigating the influence of dissipation on quantum tunneling and has a wide range of applications.[1, 2] Over decades the model has been studied by various methods,[1] like path integral,[3] renormalization group calculation,[4, 5] variational calculation,[6, 7, 8, 9, 10, 11, 12] and the numerical renormalization group(NRG) calculation,[13] etc.. One important issue is to study the cross-over from the delocalized to localized phases as the dissipation increases. Most of the studies are concentrated on the Ohmic dissipation case which is considered as corresponding to real physical systems and the cross-over picture is well understood. On the other hand, the situation for the sub-Ohmic dissipation, which is of less physics interest but still important for a well understanding of the spin-boson model, has some confusions. Renormalization group calculation shown that quantum tunneling is totally suppressed by dissipation for any non-zero sub-Ohmic coupling at T=0,[1, 4] while different conclusion was found by mapped the spin-boson model to an Ising model[14] and using the well-known result for Ising model.[15] The sub-Ohmic case was also studied by using infinitesimal unitary transformation and the cross-over was found to be discontinuous.[16] Recently, the NRG calculation, which is considered as a powerful tool for investigation of the Kondo model and its generalizations, confirmed the delocalized to localized phase cross-over in sub-Ohmic dissipation case and the cross-over is identified as continuous.[13] Variational calculation has been used to study the spin-boson model with a Ohmic bath and the result of cross-over boundary is in good agreement with the renormalization group calculation.[8, 9, 10, 11] The variational calculation for non-zero temperature[9] was generalized to sub-Ohmic case recently and the discontinuous cross-over behavior was found to exist at non-zero-temperature.[12] Up to now, the description for this discontinuous cross-over is just limited to the discontinuous change of the tunneling splitting at the cross-over point, while a scenario for such a discontinuous cross-over is still lacking. According to Ginzburg-Landau theory[17, 18], the evolution of the free energy around the critical point for the first order(discontinuous) phase transition is rather complicated and merely a discontinuous change of order parameter at the cross-over point is certainly no enough for a complete description of this discontinuous transition. In this paper, we present further analysis on this discontinuous cross-over by examining the evolution of the solutions of the self-consistent equation derived from the variational calculation. It is found that the evolution of the solutions near the phase boundary is consistent with the general picture of the first order phase transition. Basing on the constructed picture, it is shown that the critical points determined in the general way are not thermodynamically critical points and the true critical point is calculated. The arrangement of the paper is as follows. In the next section, the model and a brief explanation on variational calculation are presented. In section III we present analysis on the discontinuous phase transition by comparing the evolution of the solutions of the self-consistent equation for Ohmic and sub-Ohmic dissipation cases near the critical point. Conclusions and discussion are given in the last section.

II. THE MODEL AND VARIATIONAL CALCULATION

The Hamiltonian of the spin-boson model is given by(setting $\hbar = 1$)[1, 2]

$$H = \frac{\epsilon}{2}\sigma_z + \frac{\Delta}{2}\sigma_x + \sum_k b_k^\dagger b_k \omega_k + \sigma_z \sum_k c_k (b_k^\dagger + b_k), \quad (1)$$

where $\sigma_i (i = x, y, z)$ is the Pauli matrix, $b_k(b_k^\dagger)$ is the annihilation(creation) operator of the kth phonon mode with energy ω_k and c_k is the coupling parameter. The main interest of the present paper will be the zero temperature so we set the bias $\epsilon = 0$ in the following. It is known that the solution of this model is determined by the so-called the bath spectral function(density) defined

as[1, 2]

$$J(\omega) = \pi \sum_k c_k^2 \delta(\omega - \omega_k). \quad (2)$$

Generally $J(\omega)$ is characterized by a cut-off frequency ω_c and has a power-law form, i.e.,

$$J(\omega) = \frac{\pi}{2} \alpha \omega^s / \omega_c^{s-1}, \qquad 0 < \omega \le \omega_c, \quad (3)$$

where α is a dimensionless coupling strength which characterizes the dissipation strength. Parameter s specifies the property of the bath, $s = 1$ is the case of Ohmic dissipation and $0 \le s < 1$ the sub-Ohmic dissipation case. It should be noted that $J(\omega)$ can take some different forms,[1, 12] like $J_1(\omega) = \frac{\pi}{2}\alpha\omega^s/\omega_c^{s-1} e^{-\omega/\omega_c}$ and $J_2(\omega) = \frac{\pi}{2}\alpha\omega^s/\omega_s^{s-1}$ with $\omega_c \to \infty$, while we find that the solution is almost the same in sub-Ohmic case(see below).

As one can see from the Hamiltonian given in Eq.(1), when $\Delta = 0$ the localized phase is stable since in this case we have $[\sigma_z, H] = 0$. This result implies that the coupling to phonon bath alone cannot lead to tunneling and thus this problem can be treated approximately in the way without coupling to the bath as given in the quantum mechanics textbook.[19] To ensure the tunneling is small which is a precondition of our treatment, the following calculation is restricted to the condition $\Delta/\omega_c \ll 1$. We denote the eigen-states of spin-up(down)-plus-bath as $|\uparrow\rangle|\phi_+\rangle(|\downarrow\rangle|\phi_-\rangle)$, where $|\phi_\pm\rangle$ represent the eigen-state of the phonon bath without tunneling. When the tunneling is taken into account, the eigen-state of the whole system can be approximately given by[19]

$$|\Phi_\pm\rangle = (|\uparrow\rangle|\phi_+\rangle \pm |\downarrow\rangle|\phi_-\rangle)/\sqrt{2}, \quad (4)$$

then the tunneling splitting in the presence of dissipation is

$$\Delta' = \langle\Phi_+|H|\Phi_+\rangle - \langle\Phi_-|H|\Phi_-\rangle = \Delta\langle\phi_+|\phi_-\rangle, \quad (5)$$

a well known result that Δ' is determined by the overlap integral of the phonon ground states.[10, 11] In the absence of tunneling(i.e., $\Delta = 0$), Hamiltonian (1) can be diagonalized by a well-known displaced-oscillator-transformation and the phonon ground states are the so-called displaced-oscillator-states[20]

$$|\phi_{d\pm}\rangle = \exp\{\pm \sum_k \frac{c_k}{\omega_k}(b_k - b_k^\dagger)\}|0\rangle,$$

where $|0\rangle$ is the vacuum state of the phonon. The essence of the variational calculation is that, in the presence of tunneling, the phonon ground states are suggested to still have the same from, i.e.,

$$|\phi_\pm\rangle = \exp\{\pm \sum_k g_k(b_k - b_k^\dagger)\}|0\rangle, \quad (6)$$

but leaving the parameter g_k to be determined from the condition that the ground state energy of the whole system is a minimum with respect to g_k. Substituting the above equation to Eq.(4), the ground state energy of the whole system is found to be

$$E[g_k] = \sum_k(\omega_k g_k^2 - 2c_k g_k) - \frac{1}{2}\Delta \exp\{-2\sum_k g_k^2\}, \quad (7)$$

which is a functional of g_k, then $\frac{\delta E}{\delta g_k} = 0$ leads to

$$g_k = \frac{c_k}{\omega_k + \Delta\exp\{-2\sum_k g_k^2\}}, \quad (8)$$

the tunneling splitting, by Eq.(5), is given by

$$\Delta' = K\Delta, \qquad K = F[g_k] \equiv \exp\{-2\sum_k g_k^2\}. \quad (9)$$

Using Eq.(8) and the definition of the spectral function, we find that K is determined by the following self-consistent(or variational) equation

$$K = f(K), \qquad f(K) \equiv \exp\{-\alpha \int_0^1 \frac{x^s\, dx}{[x + (\Delta/\omega_c)K]^2}\}. \quad (10)$$

Such a kind of self-consistent equation has been derived in previous works[7, 8, 9, 10, 11, 12] and it plays an important role in dealing with the cross-over from the delocalized to localized phases. It is easy to see that $K = 0$ is the trivial solution of Eq.(10) and this solution represents the localized phase. When the coupling strength α is large enough, $K = 0$ is the only solution of the self-consistent equation, while as α decreases to some value α_c, the self-consistent equation begins to have, in addition to the trivial solution, non-zero solutions, then α_c is identified as the critical point at where the cross-over from the localized($K = 0$) to delocalized($K > 0$) phases happens. This is the general way to determine the phase boundary used in previous works.[8, 9, 10, 11, 12]

In the case of Ohmic dissipation, i.e., $s = 1$, the self-consistent equation can be solved analytically and the phase boundary is found to be $\alpha_c = 1$ in the case of $\Delta/\omega_c \ll 1$, in agreement with the renormalization group calculation.[8, 9, 11] In the case of sub-Ohmic dissipation, the self-consistent equation can be solved numerically and the phase boundary between the localized($K = 0$) and delocalized($K > 0$) phases determined in this way is shown in Fig.1. The result by using different spectral functions, i.e., $J_1(\omega)$ and $J_2(\omega)$, are also shown in the inset. Our result shows that, for $\Delta/\omega_c \ll 1$, the phase boundary is almost the same for all three spectral functions as $s \le 0.7$, while α_c is a little bit lower for $J_2(\omega)$ when $s > 0.7$. Also, it is found that the relation between the critical coupling α_c and Δ/ω_c has a simple power-law form $\alpha_c \propto (\Delta/\omega_c)^{1-s}$ as found by NRG calculation.[13] Notably, such a relation can be deduced from Eq.(16) in ref.[16] by using the spectral function given here.[21] However, as we shall show in the next section, the α_c determined in this way for sub-Ohmic case is not thermodynamically the critical point, but just the the limit of metastability for superheating of the first order phase transition.[18]

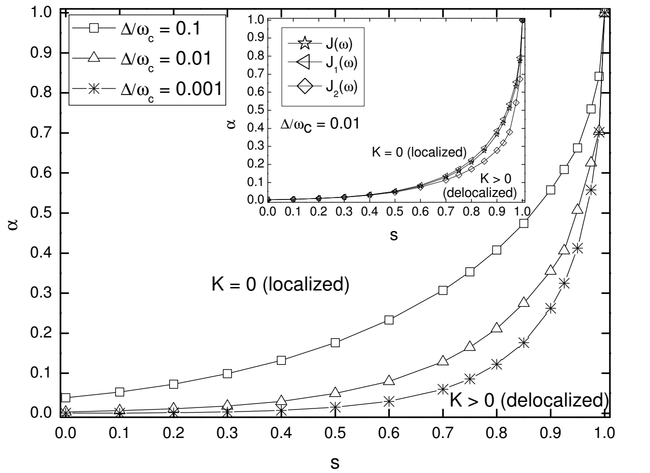

FIG. 1: Phase boundary determined by α_c for various Δ/ω_c. The inset shows the comparison with the result by using different spectral function $J_1(\omega)$ and $J_2(\omega)$(see the text) in the case of $\Delta/\omega_c = 0.01$.

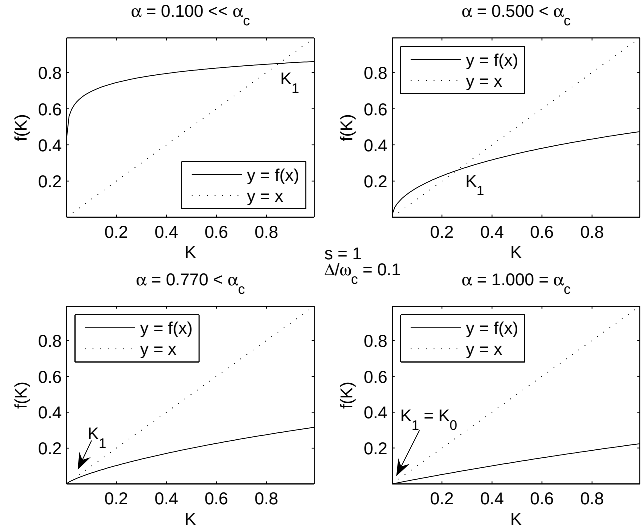

FIG. 2: Evolution of the solutions of Eq.(10) with the increase of coupling strength α for $\Delta/\omega_c = 0.1$ in the case of Ohmic dissipation $s = 1$.

III. THE DISCONTINUOUS CROSS-OVER IN SUB-OHMIC CASE

Now we turn to present a scenario for such a discontinuous cross-over from the delocalized to localized phases in sub-Ohmic case. The key point is to examine the evolution of the solutions of the self-consistent equation with the coupling strength α near the phase boundary. For clarity, we first see what happens in the Ohmic case. Fig.2 shows the evolution of the solutions of Eq.(10) with the increase of α in Ohmic dissipation case. When $\alpha > \alpha_c$, we have the trivial solution only, while a non-zero solution($K_1 \neq 0$) appears for $\alpha < \alpha_c$. As one can see from the figure, the non-zero solution K_1 continuously tends to 0 as α approaches α_c. This is consistent with the picture of a continuous(second order) transition: [17, 18] above the critical point($\alpha > \alpha_c$), there is only one stable phase(one energy minimum located at some g_{k0} satisfying $F[g_{k0}] = 0$ in the present case), below the critical point, this stable phase becomes unstable($E[g_{k0}]$ becomes the maximum of the energy) and a second stable phase appears($E[g_{k1}]$ is the new energy minimum, where $F[g_{k1}] = K_1 > 0$), the cross-over behavior is continuous.

The situation for the sub-Ohmic dissipation case is qualitatively different. As shown in Fig.3, when $\alpha < \alpha_c$, there are *two* non-zero solutions of Eq.(10)($K_2 > K_1 \neq 0$) in additional to the trivial solution.[22] As the coupling strength α increases, K_2 decreases while K_1 increases and tends to meet K_2 as α approaches α_c. At $\alpha = \alpha_c - 0$, we have $K_1 = K_2 = K_0 \neq 0$ and at this point K_0 is the point of tangency for the line $y = x$ and curve $y = f(x)$. At $\alpha = \alpha_c + 0$, the solution K_0 disappears *suddenly* and only the trivial solution is found. The α-dependence of the non-zero solutions of Eq.(10) for Ohmic and sub-Ohmic dissipation cases are shown in Fig.4 where one can see

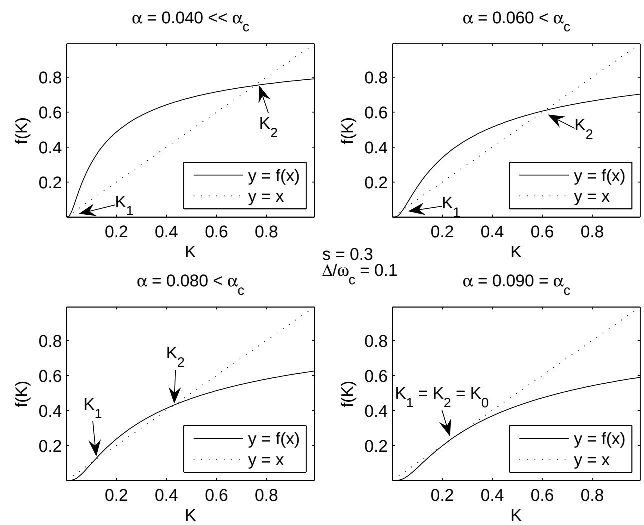

FIG. 3: Evolution of the solutions of Eq.(10) with the increase of coupling strength α for $\Delta/\omega_c = 0.1$ in the case of sub-Ohmic dissipation $s = 0.3$.

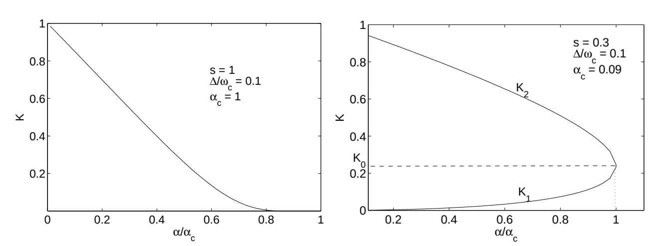

FIG. 4: The α-dependence of the non-zero solution of Eq.(10) for $s = 1$(left) and $s = 0.3$(right). As $\alpha/\alpha_c \to 1$, the non-zero solution of $s = 1$ approaches 0 continuously, while for $s = 0.3$, the non-zero solution jumps from $K_0 \neq 0$ to 0.

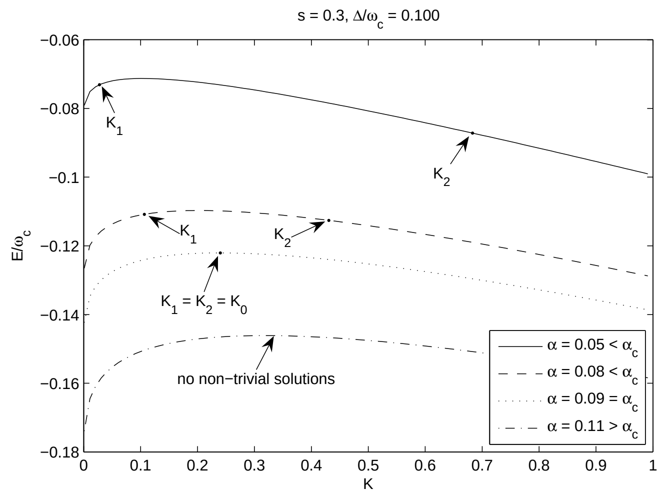

FIG. 5: Evolution of the K-dependence of the ground state energy E with coupling strength α for sub-Ohmic case($s = 0.3$) when $\Delta/\omega_c = 0.1$.

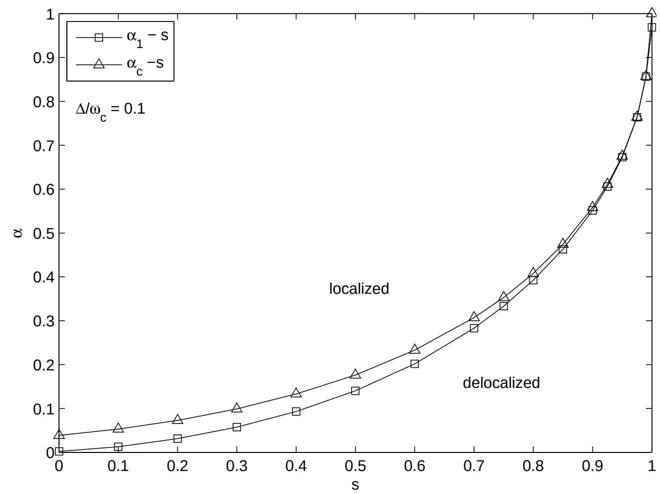

FIG. 7: The phase boundary determined by α_c and α_1 in the case of $\Delta/\omega_c = 0.1$.

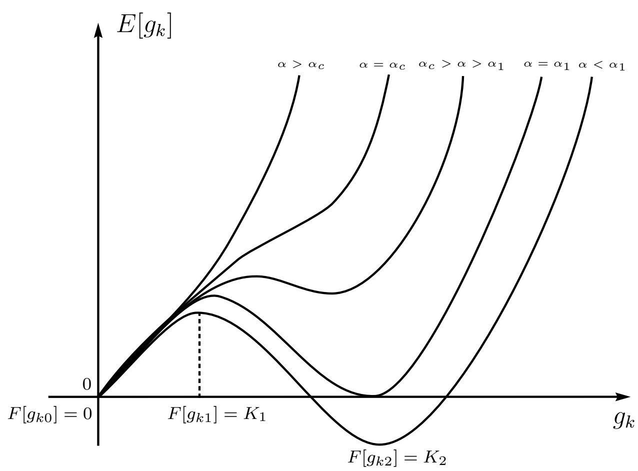

FIG. 6: The evolution of the energy extrema with the coupling strength α for the sub-Ohmic case. Thermodynamically the cross-over point is α_1, while α_c is just the point where the second minimum begins to develop.

the qualitatively different cross-over behavior. The result of sub-Ohmic dissipation case clearly shows that the cross-over is discontinuous since the non-zero solution of Eq.(10) and thus the tunneling splitting Δ' changes discontinuously at the point $\alpha = \alpha_c$. Such a behavior was found before[12, 16] and took as the evidence for a discontinuous transition since the tunneling splitting has a physics meaning of the order parameter.

What we want to emphasize here is the two non-zero solutions when $\alpha < \alpha_c$. Physically we need to know which solution is stable and the meaning of the second non-zero solution. As one can see from Fig.4(right), the non-zero solution K_1 increases with α, one can intuitively conclude that K_1 is unstable since physically the tunneling splitting should decrease with α. Basing on the variational calculation, we cannot make further analysis on the stability of the solution, so we turn to energy analysis, i.e., to see which solution is energy preferable. Typical evolution of the $E-K$ curve with α is shown in Fig.5. The result shows that, we have $E(K_1) > E(0)$ and $E(K_1) > E(K_2)$ when $\alpha \ll \alpha_c$, $E(0)$ decreases while both $E(K_1)$ and $E(K_2)$ increase relatively as α increases but $E(K_1)$ is always the largest, finally $E(K_1) = E(K_2) = E(K_0)$ as $\alpha = \alpha_c$ and we have $E(0) < E(K_0)$. This implies that, both $K = 0$ and K_2 are energy preferable while K_1 is unstable when $\alpha < \alpha_c$. Such a result is consistent with the scenario of a first order transition. In the scenario of the first order transition,[17, 18] below the critical point, there are two free energy minima and a maximum lies between, while above the critical point, only one global free energy minimum survives. In the sub-Ohmic dissipation case, when $\alpha < \alpha_c$, three solutions of Eq.(10) represent the two energy minima and one energy maximum, that is, $E[g_{k0}]$ with $F[g_{k0}] = 0$ and $E[g_{k2}]$ with $F[g_{k2}] = K_2$ are the two energy minima, while $E[g_{k1}]$ with $F[g_{k1}] = K_1$ is the energy maximum lies between as shown in Fig.6. As α increases and approaches α_c, $E[g_{k1}]$ tends to meet $E[g_{k2}]$ and at the point $\alpha = \alpha_c$, these two energy extrema merge into a point of inflection at $F[g_k] = K_0$, then only one energy minimum $E[g_{k0}]$ survives when $\alpha > \alpha_c$. Based on the picture for the discontinuous phase transition, it is now clear that α_c is *not* the critical point for the cross-over to happen, but just the point where the second energy minimum begins to develop. α_c can be considered as the limit of metastability for superheating,[18] i.e., the limit of metastability for increasing the dissipation strength in the present case. Thermodynamically the critical point, as shown in Fig.6, should be α_1 where we have[17, 18]

$$E(K_2) = E(0), \tag{11}$$

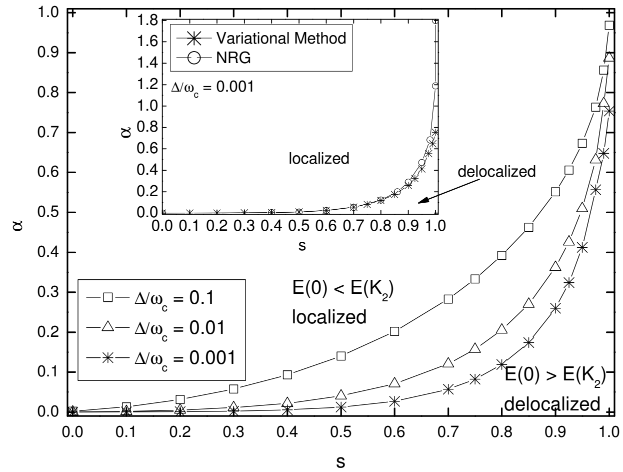

FIG. 8: The phase boundary determined by α_1 for various Δ/ω_c. The inset shows the comparison with the NRG calculation in the case of $\Delta/\omega_c = 0.001$.

from this, α_1 can be determined by Eqs.(7), (8) and (10). Comparison between the phase boundary determined by α_c and α_1 is shown in Fig.7. It is easy to see that $\alpha_1 < \alpha_c$ while the difference between α_c and α_1 decreases as s increases and tends to zero as $s \to 1$ where the transition becomes continuous. We also find that the difference between α_c and α_1 decreases with Δ/ω_c. The phase boundary deduced in this way is shown in Fig.8 which is similar to that shown in Fig.1 but with all the critical points lower. It is found that the phase boundary determined by α_1 is in good agreement with that obtained by NRG calculation when $\Delta/\omega_c \leq 0.01$.

IV. CONCLUSIONS AND DISCUSSION

In conclusion, we have study the cross-over behavior from localized to delocalized phases of a spin-boson model with a sub-Ohmic bath by variational method. By examining the evolution of the solutions of self-consistent equation (10) with the coupling strength, we are able to present the scenario of the discontinuous transition in sub-Ohmic dissipation case. Based on the constructed picture, it is shown that the α_c, at where the self-consistent equation begins to have non-zero solutions, is not thermodynamically the critical point, but just the point where the second energy minimum begins to develop. The true critical point is determined according to Ginzburg-Landau theory for the first order phase transition and the obtained phase boundary is in agreement with the NRG calculation. Our analysis shows that the cross-over behavior in spin-boson model is directly related to the evolution of solutions of the self-consistent equation derived from the variational calculation. The evolution behavior of solutions for a continuous cross-over(in Ohmic dissipation case) is qualitatively different from that of a discontinuous cross-over(in sub-Ohmic dissipation case). The present work, on one hand, provides convincing evidence for a discontinuous cross-over in sub-Ohmic case and on the other hand, demonstrates the new way to deal with the cross-over behavior in spin-boson model by the variational method.

According to the definition of stable and unstable fixed points for renormalization group,[23] geometrically one can see from Fig.3 that, both $K = 0$ and K_2 are stable fixed points while K_1 is unstable fixed point as $\alpha < \alpha_c$ in sub-Ohmic case. On the other hand, we only have one stable fixed point(i.e., K_1) and one unstable fixed point as $\alpha < \alpha_c$ in Ohmic case. This result is in agreement with the NRG calculation, [13] where 3 fixed points(2 stable and 1 unstable) were found in sub-Ohmic case while the third unstable fixed point disappeared in Ohmic case. However, the cross-over behavior in sub-Ohmic case was identified as continuous in NRG calculation, this implies further analysis is needed for seeking a deeper relation. Although the work by Kehrein and Mielke is not based on the variational calculation,[16] the cross-over behavior was studied by a self-consistent equation and the discontinuous behavior was judged by the discontinuous change of the tunneling splitting at the critical point α_c, where the self-consistent equation begins to have non-zero solutions. Some results, like the (Δ/ω_c) dependence of critical coupling α_c and the s-dependence of tunneling splitting at the critical point also show quantitative agreement with our work determined from Eq.(10) at $\alpha = \alpha_c$. This may lead to a conclusion the the critical point determined in ref.[16] is just α_c given in the present work, i.e., not thermodynamically the critical point.

The author(Chen) thanks Dr. N. H. Tong for supplying the data of phase diagram by NRG calculation. This work was supported by a grant from the Natural Science Foundation of China under Grant No. 10575045.

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